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ABSTRACT

$CePdIn_2$ is found to crystallize in the orthorhombic space group *Cmcm* (Z=4) with a = 4.6210(9) Å, b = 10.694(2) Å, and c = 7.455(2) Å. Single crystal X-ray data were refined to R = 0.0459 (wR_2 = 0.0666), with 255 independent reflections and 16 variables. The structure adopts the BRe_3 structure type and is the first known Ce-containing member. Magnetic measurements indicate that $CePdIn_2$ undergoes a ferromagnetic phase transition with a T_c near 10 K. The electrical resistivity of $CePdIn_2$ shows metallic behavior with a small anomaly at the magnetic phase transition.

INTRODUCTION

Over the past 20 years, research in ternary cerium intermetallics has grown substantially as interesting strongly correlated electron systems have been observed (1,2,3). While much progress has been made in understanding the origin of these effects, this knowledge is insufficient to predict new compounds which exhibit these phenomena.

However, as discussed by Fisk et al. (4), the chemical composition of the interesting Ce compounds includes mostly elements in the late transition metal and early p block columns. In particular, in the Ce-Pd-In ternary phase diagram, there are a number of interesting correlated electron materials such as $CePd_3$ (5), $CeIn_3$ (6), and CePdIn (7).

Motivated by the unusual materials found in this system as well as more recently discovered compounds (8), we have been searching for other new ternaries in this phase space (9). Here, we report the structure and properties of a new compound, $CePdIn_2$.

EXPERIMENTAL

Sample Preparation

$CePdIn_2$ was synthesized by arc-melting stoichiometric amounts of the elements on a water-cooled, Ta coated copper hearth under a flow of Ti-gettered Ar (Centorr Furnaces, Model 2B-20). The arc-melted beads were flipped over and remelted repeatedly to increase homogeneity. Mass losses after arc-melting were less than 0.5%.

The elements used were all at least of purity 99.9%. The cerium was further purified by vacuum melting into a water-cooled copper cup, leaving behind much of the outer oxide coat often present on Ce pieces.

The arc-melted beads were then placed in tantalum tubing and sealed in quartz under vacuum. The beads were then heated at 825 °C for one week.

Structure determination

Preliminary structure characterization was done with electron and x-ray diffraction of finely ground powder. Electron diffraction patterns were obtained using powder suspended on holey carbon coated grids in a double tilt holder in a JEOL 1200 EX transmission electron microscope. The powder was also studied by X-ray diffraction using a Scintag XDS 2000 diffractometer with Cu K_α radiation. The diffraction data indicated an orthorhombic cell of approximate dimensions 4.621 x 10.692 x 7.450 Å and C-centering.

Shards of lightly cracked beads were mounted and screened for crystal quality using precession camera photos. Single crystal data were collected on a Siemens P4 four-circle diffractometer in the θ-2θ mode from $-1 \le h \le 6$, $-1 \le k \le 13$, and $-1 \le l \le 9$. The lattice constants for the cell were a = 4.6210(9) Å, b = 10.694(2) Å, and c = 7.455(2) Å, in good agreement with the powder data. Three check reflections were measured every 50 reflections, and they showed no evidence of crystal decomposition or movement on the fiber. An empirical psi-scan absorption correction was applied to the data, yielding an $R_{int} = 0.0305$. The semi-invariants representation program SIR92 (10) was used to generate a model for the structure which was refined with XL from the SHELXTL

version 5γ program (11). The final structure R values were $wR_2 = 0.0666$ and $R_1 = 0.0459$ for all data and $wR_2 = 0.0614$ and $R_1 = 0.0310$ for $I > 2\sigma(I)$. The MISSYM algorithm (12) detected no further symmetry elements than those expected for Cmcm.

Crystal structure data, values of the atomic parameters, and anisotropic displacement parameters are listed in Tables 1, 2, and 3. The atomic positions are presented both in accordance with previous BRe_3 structure literature and also in the standard format as determined by the program STRUCTURE TIDY (13). This program standardizes inorganic structures to help identify similar structures, obscured by differences in the reporting of crystal data.

Additional structure information, including structure amplitudes, is available as supplementary material.[1]

Physical property measurements

The magnetic susceptibility of $CePdIn_2$ was measured using a Faraday balance on coarsely ground, loose powder. The field dependence of the susceptibility at room temperature from 2.1 kG to 14.6 kG showed variations of less than 1%, indicating the absence of ferromagnetic impurities. Temperature dependent data from 4 to 325 K were collected in a field of 10 kG. Platinum was used as a calibration standard. The measured room temperature susceptibility of Pt χ(293 K) was 1.030×10^{-6} emu/g, in good agreement with a literature value of 1.035×10^{-6} emu/g (14).

Electrical resistivity was measured using standard four probe AC techniques. The contacts were ohmic by linearity of the I-V curve. The

resistivity sample was bar-shaped, cut with a string saw from a bead after heat treatment.

RESULTS AND DISCUSSION

Structural Aspects

The structure of $CePdIn_2$ is isotypic with the rare earth intermetallics (Y,Gd, Tb, Dy)$NiIn_2$ (15), (Y,Tb-Lu)$NiGa_2$ (16), (Y, Tb-Lu)$PdGa_2$ (17), and (Y, Tb-Lu)$NiAl_2$ (18). Thus, the structure type was previously known only for compounds containing the smaller rare earth atoms.

As shown in Figure 1, the structure can be described as a staggered net of trigonal prisms. Each prism is composed of four In atoms and two Ce atoms centered by a Pd atom.

Selected bond distances are listed in Table 4. The bond distances indicate that the chemical environment of the atoms is more complicated than emphasized in Figure 1. Figure 2 shows the coordination polyhedra around each of the atoms as determined by the principle of maximal gap in near neighbor distances (19). All resulting distances are short enough to be considered as bonding to the central atom.

As shown in Figure 2a, the 13-coordinate environment around the Ce can be described as a distorted pentagonal prism of eight In atoms and two Pd atoms with two In atoms and one Pd atom capping three square faces of the prism. The Pd environment of nine neighbors, shown in Figure 2b, consists of a trigonal prism of four In atoms and two Ce atoms, tricapped by two In

atoms and one Ce atom. The coordination geometry of In to its 12 neighbors is irregular and is depicted in Figure 2c. It consists roughly of Ce atoms in square pyramidal coordination and In atoms in tetrahedral coordination about the central In. Three Pd atoms complete the coordination polyhedron.

The complicated polyhedra suggest that size constraints strongly limit the formation of the BRe_3 structure type. An unsuccessful attempt at making $CeNiIn_2$ underscores this probable steric limitation. The larger Pd and In atoms are perhaps necessary to stabilize the structure for the larger rare earth Ce atom. To date, the presented structure is the only known Ce or Pd-In example for this structure type.

Magnetic properties

Figure 3 shows the inverse magnetic susceptibility for $CePdIn_2$ upon heating the powder sample from 4.2 K. The data were fit to the Curie-Weiss law: $\chi = \chi_0 + \dfrac{C}{T-\theta}$.

The fit parameters were selected by choosing a temperature range of fit, fixing θ, and then determining C and χ_0 using standard analysis techniques (20). θ was varied, and for each choice, a fractional variance σ was calculated. The final parameters were chosen to minimize σ over the largest temperature range.

These parameters were found to be $\chi_0 = 2.6 \pm 0.4 \times 10^{-7}$ emu/g, C = $1.60 \pm 0.02 \times 10^{-3}$ emu-K/g, and a ferromagnetic $\theta = 16.5 \pm 1.5$ K for the temperature

range of 75 to 325 K with a $\sigma = 1.5 \times 10^{-3}$. At temperatures below 75 K, some deviations from the Curie-Weiss law occur, most likely due to crystal field effects. The Curie constant corresponds to a moment of $2.47 \pm 0.02\ \mu_B$ which is very close to the free ion value of $2.54\ \mu_B$ for Ce^{+3}. Hence, it appears that in $CePdIn_2$, the Ce is trivalent, with ferromagnetic exchange. We can estimate a transition temperature of ≈ 10 K from the inflection point of the χ vs temperature curve.

As shown in Figure 4, the field dependence of the low temperature susceptibility is consistent with a ferromagnetically ordered material. Fitting the χ vs $1/H$ curve to a straight line, we obtain a magnetization at 4.2 K of 1.6 μ_B vs the expected $gJ = 2.14\ \mu_B$ for completely oriented Ce^{+3} ions in a $J=5/2$ state. The deviation from the expected value may indicate that there is some canting of the spins in the ordered state or more likely that crystal field splitting reduces the ground state moment.

The existence of ferromagnetism in this system agrees well with the empirical observations of Sereni and Kappler (21). They found that ferromagnetic behavior is often present in systems with Ce-Ce nearest neighbor distances between 3.7 and 4.1 Å. In $CePdIn_2$ this distance is 4.063 Å.

Electrical properties

Resistivity data from room temperature to 4.2 K are shown in Figure 5. The magnitude of the resistivity and its monotonic decrease with temperature down to ≈ 20 K indicate metallic conduction. At roughly 10 K,

there is a kink in the resistivity, most likely due to a coupling of the carriers to the ordering Ce moments.

Note that the resistivity decreases more rapidly below 10 K than just above, indicating that spin-disorder scattering may be playing a role at higher temperatures. Below the ferromagnetic transition, this extra scattering is expected to die out as the moments order. This behavior is similar to that observed in other rare earth intermetallic compounds such as NdAuAl (22) and GdNiGe (23).

CONCLUSIONS

We have synthesized a new ternary intermetallic compound, $CePdIn_2$, the first known Ce containing member of the BRe_3 structure type. From the magnetic and electrical properties, we conclude that $CePdIn_2$ is a ferromagnet with a T_c of about 10 K. It appears that the Ce moments do not interact strongly with the conduction electrons, as we see little evidence of Kondo-like magnetic or transport behavior.

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TABLE 1

Crystal Data and Structure Refinement for $CePdIn_2$

Empirical formula	$CePdIn_2$
Formula weight	476.16
Diffractometer type	Siemens P4 four-circle
Radiation	Graphite monochromated MoK_α, λ=0.71073 Å
Temperature	293(2) K
Scan type	θ-2θ
Crystal system	Orthorhombic
Space group	Cmcm (No. 63)
Unit cell dimensions	a = 4.6210(9) Å b = 10.694(2) Å c = 7.455(2) Å
Volume	368.40(13) $Å^3$
Z	4
Density (calculated)	8.585 g/cm^3
Absorption coefficient	29.012 mm^{-1}
F(000)	808
Crystal size	0.19 x 0.05 x 0.04 mm
θ range for data collection	3.81° to 27.48°
Index ranges	$-1 \le h \le 6$, $-1 \le k \le 13$, $-1 \le l \le 9$
Reflections collected	391
Independent reflections	255 (R_{int} = 0.0305)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.984 and 0.509
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	255/0/16
Goodness-of-fit on F^2	1.089
Final R indices ($I>2\sigma(I)$)	R_1 = 0.0310, wR_2 = 0.0614
R indices (all data)	R_1 = 0.0459, wR_2 = 0.0666
Largest diff. peak and hole	2.547 and -1.546 $eÅ^{-3}$

TABLE 2

Atomic Coordinates[a] and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $CePdIn_2$

	x	y	z	U(eq)
In in 8(f)	0.0 [0.0]	0.3612(1) [0.1388]	0.0506(1) [0.0506]	11(1)
Ce in 4(c)	0.0 [0.0]	0.0756(1) [0.4244]	0.25 [0.25]	10(1)
Pd in 4(c)	0.0 [0.0]	0.7931(2) [0.7069]	0.25 [0.25]	11(1)

[a]Coordinates in brackets are in STRUCTURE TIDY format.

TABLE 3

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $CePdIn_2$

	U_{11}	U_{22}	U_{33}	U_{23}	$U_{13}=U_{12}$
Pd	9(1)	12(1)	10(1)	0	0
Ce	10(1)	11(1)	11(1)	0	0
In	11(1)	13(1)	8(1)	1(1)	0

TABLE 4

Interatomic Bond Distances (Å) for $CePdIn_2$

Ce	1Pd	3.021(3)
	2Pd	3.278(2)
	4In	3.2891(9)
	2In	3.396(2)
	4In	3.5786(13)
Pd	1Ce	3.021(3)
	2Ce	3.278(2)
	2In	2.783(2)
	4In	2.8421(9)
In	2Ce	3.2891(9)
	1Ce	3.396(2)
	2Ce	3.5786(13)
	1Pd	2.783(2)
	2Pd	2.8421(9)
	1In	2.973(2)
	1In	3.064(2)

LIST OF FIGURE CAPTIONS

FIG. 1. Structure of $CePdIn_2$ illustrating trigonal prismatic coordination around the Pd atoms.

FIG. 2. Local coordination environments around a) Ce b) Pd and c) In atoms. The dark lines indicate the pentagonal and trigonal prismatic units in the Ce and Pd coordination polyhedra.

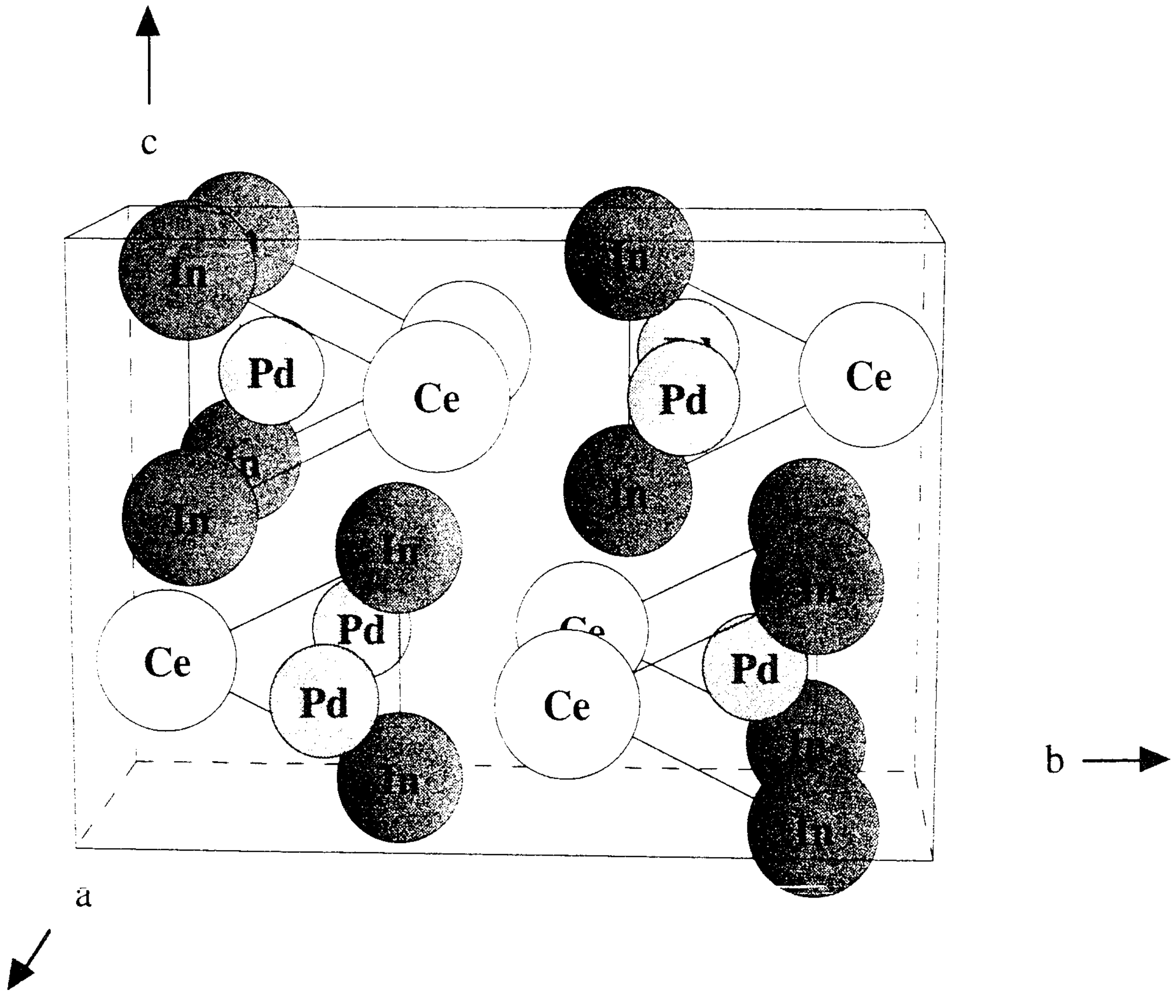
FIG. 3. Inverse magnetic susceptibility as a function of temperature. Inset shows susceptibility vs temperature for $T < 50$ K.

FIG. 4. Magnetic susceptibility vs inverse field at 4.2 K.

FIG. 5. Electrical resistivity as a function of temperature. Inset shows resistivity for $T < 25$ K.

LIST OF FOOTNOTES

[1] See NAPS document No. __ for __ pages of supplementary material. Order from ASIS/NAPS. Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, NY 10163. Remit in advance $4.00 for microfiche copy or for photocopy, $7.75 up to 20 pages plus $0.30 for each additional page. All orders must be prepaid. Institutions and Organizations may order by purchase order. However, there is a billing and handling charge for this service of $15. Foreign orders add $4.50 for postage and handling, for the first 20 pages, and $1.00 for additional 10 pages of material, $1.50 for postage of any microfiche orders.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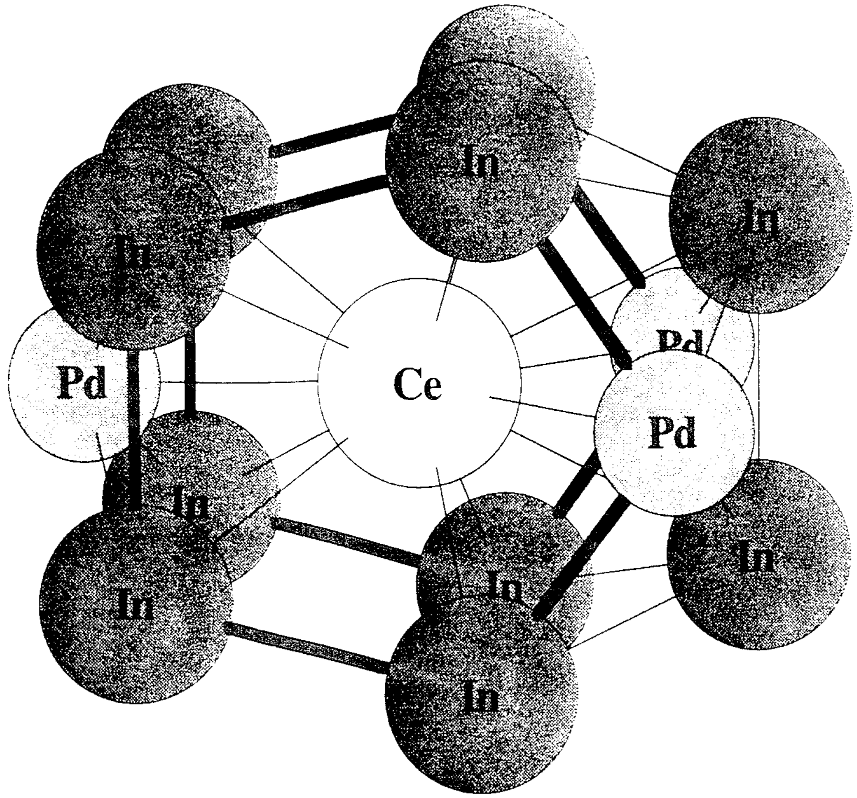
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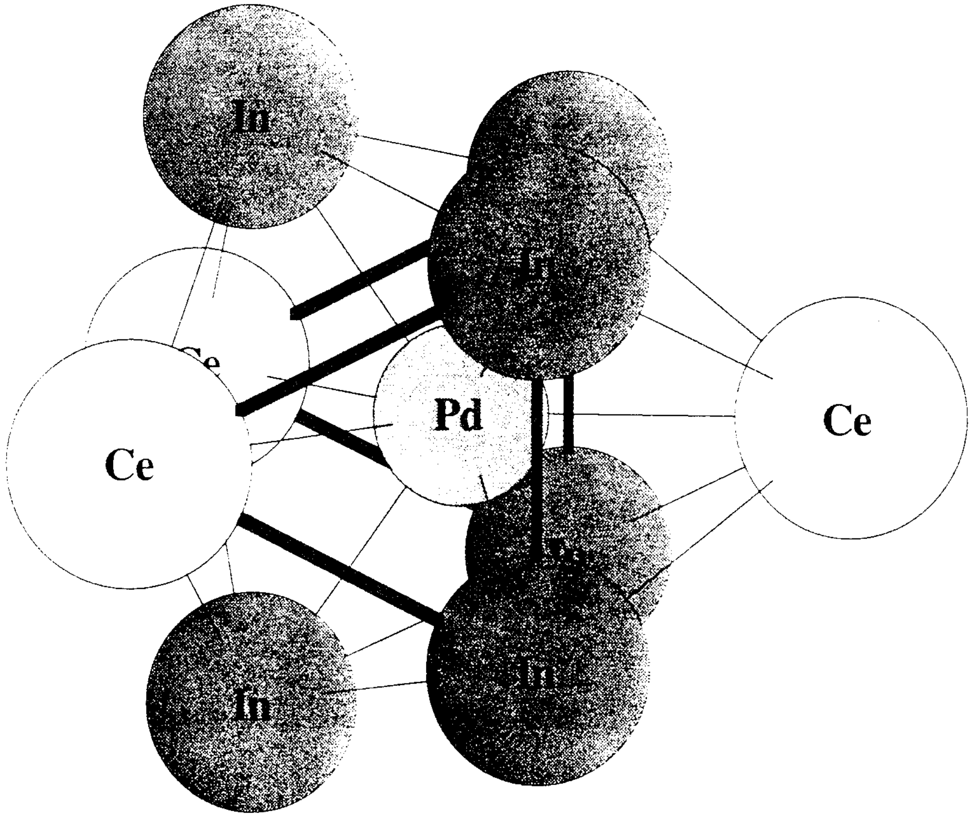
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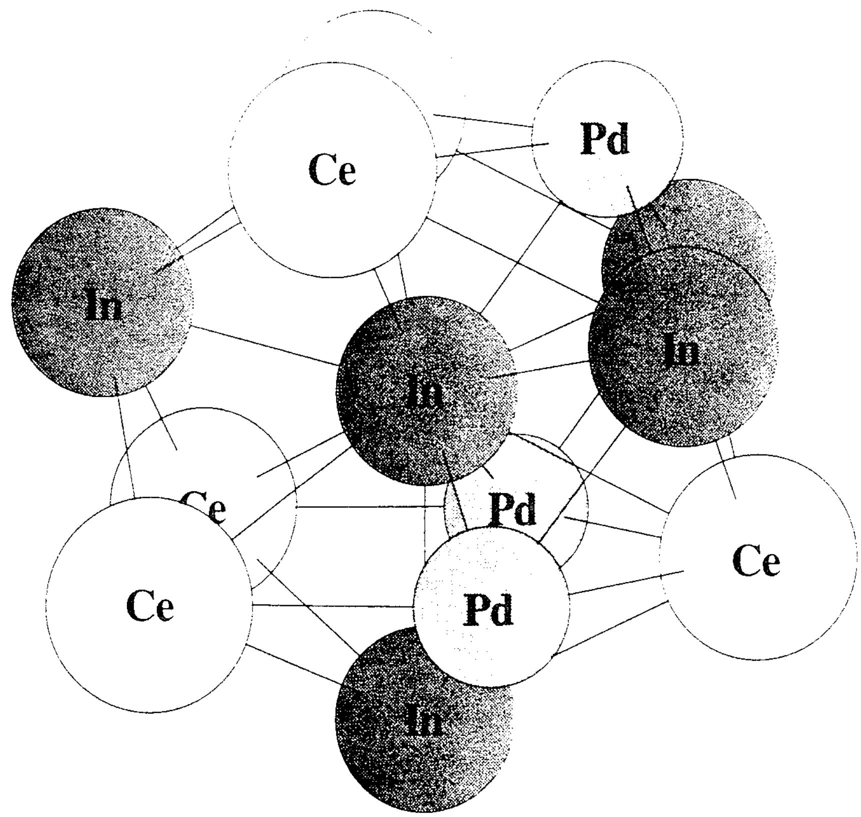
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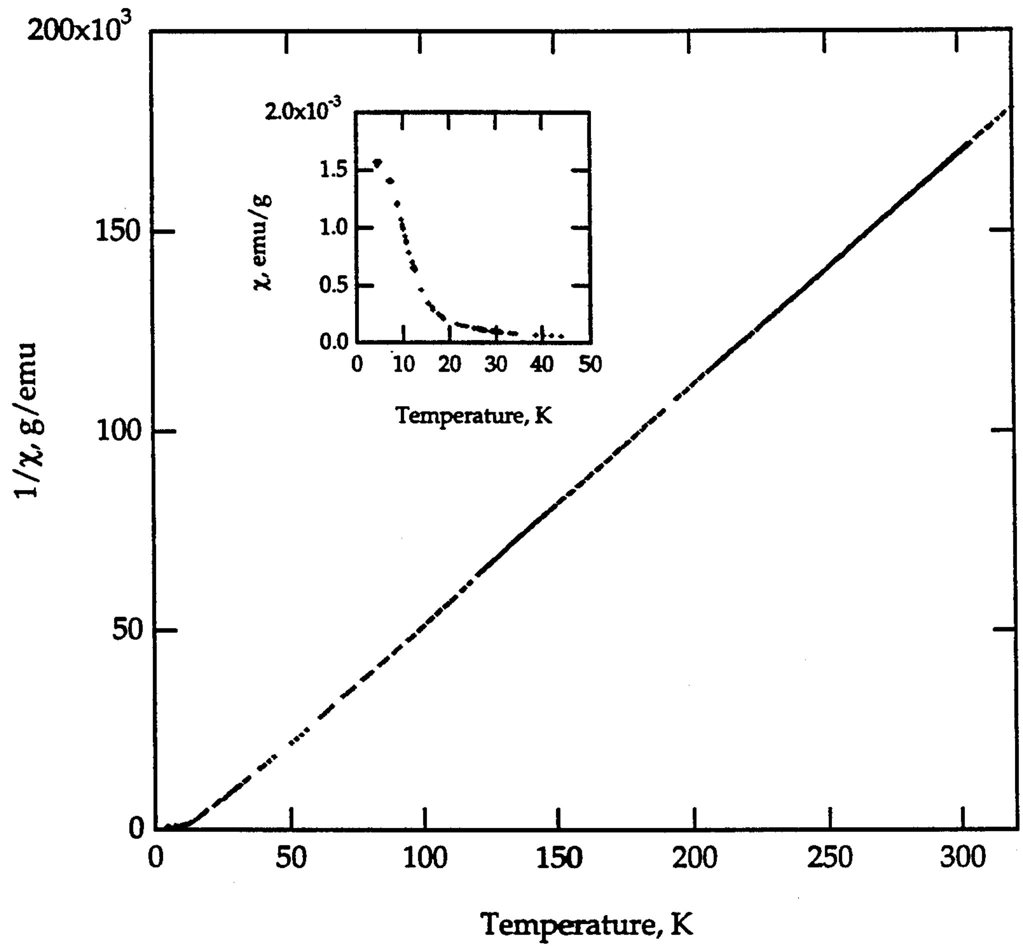
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1/χ, g/emu
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100
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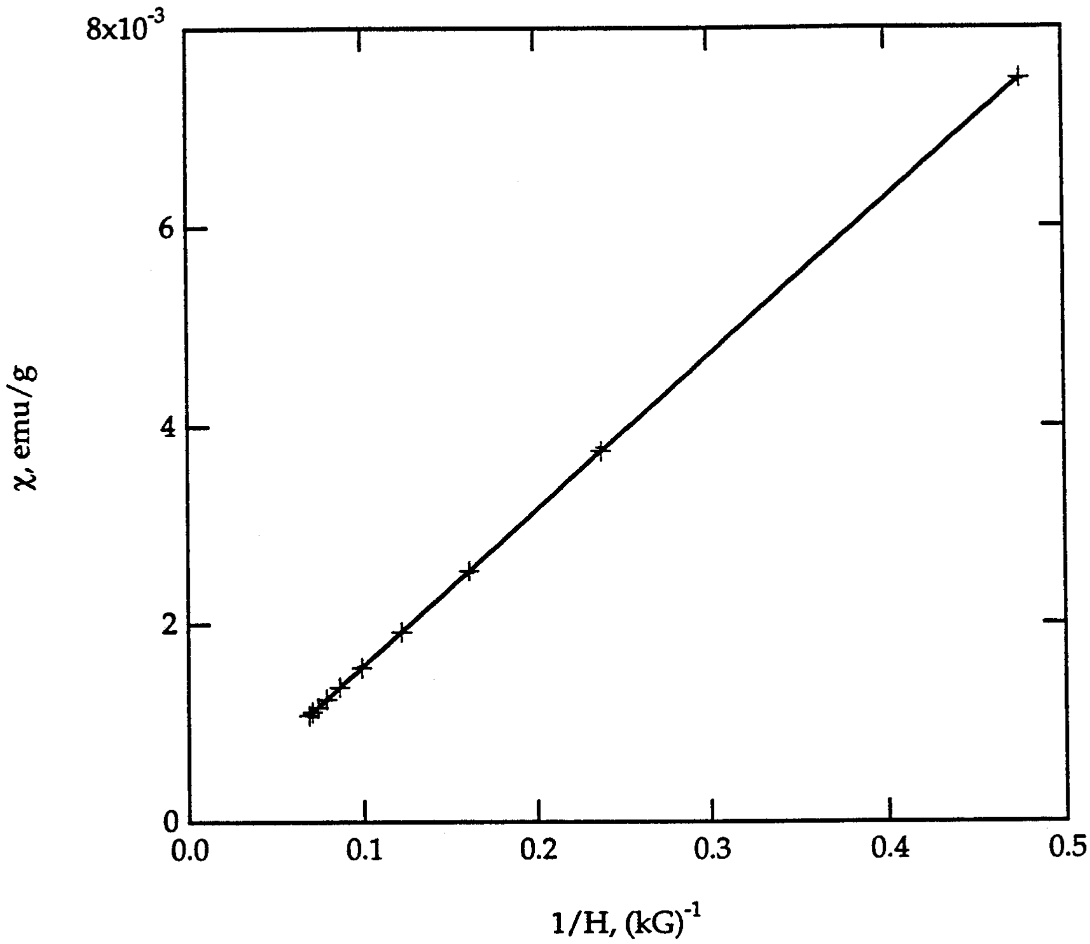

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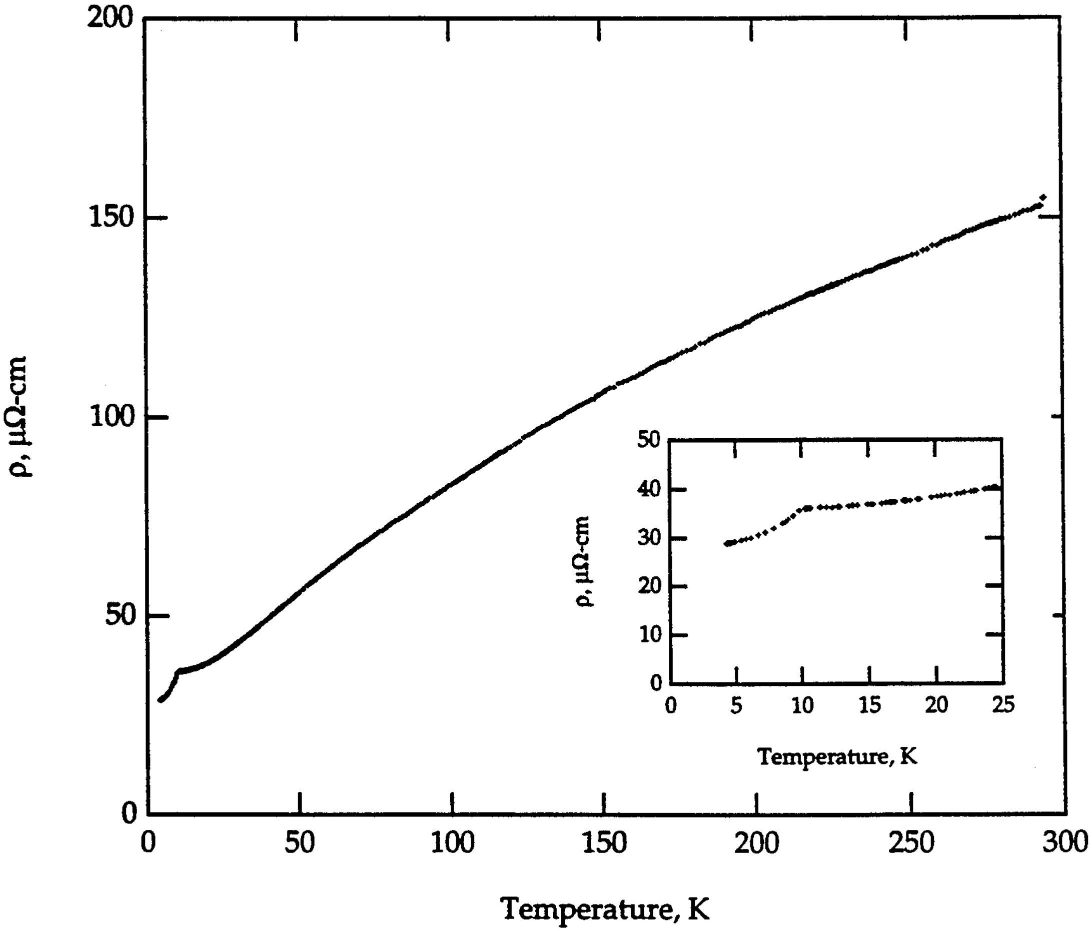

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Temperature, K
ρ, μΩ-cm
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40
30
20
10
0
0
5
10
15
20
25
Temperature, K

Supplementary information: observed and calculated structure factors

h	k	l	10Fo	10Fc	10s
2	0	0	6254	6015	40
4	0	0	3912	3868	31
6	0	0	2435	2462	24
1	1	0	124	45	36
3	1	0	135	62	134
5	1	0	171	99	98
0	2	0	858	834	16
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4	2	0	408	375	46
1	3	0	1873	1910	39
3	3	0	1329	1353	31
5	3	0	857	845	29
0	4	0	2752	2798	45
2	4	0	2315	2318	38
4	4	0	1568	1556	32
1	5	0	966	970	22
3	5	0	677	683	33
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2	2	2	286	242	49
4	2	2	0	186	1
1	3	2	2740	2738	29
3	3	2	1961	1966	37
5	3	2	1240	1281	26
0	4	2	2219	2216	46
2	4	2	1838	1848	46
4	4	2	1254	1246	30
1	5	2	685	649	20
3	5	2	558	514	40
5	5	2	275	343	116
0	6	2	2315	2295	46
2	6	2	1979	2005	45
4	6	2	1442	1465	30
1	7	2	544	521	33
3	7	2	472	460	52
5	7	2	296	366	120
0	8	2	2656	2685	41
2	8	2	2409	2395	37
4	8	2	1753	1808	28
1	9	2	0	47	1
3	9	2	197	39	197
0	10	2	1694	1693	38
2	10	2	1560	1536	34
1	11	2	769	764	28
3	11	2	590	637	64
0	12	2	628	630	47
2	12	2	574	575	60
1	13	2	933	875	27
1	1	3	2292	2277	20
3	1	3	1628	1631	26
5	1	3	1046	1063	20
0	2	3	3103	3041	39
2	2	3	2481	2567	42
4	2	3	1785	1777	29
1	3	3	1286	1305	21
3	3	3	995	1018	25
5	3	3	764	733	34
0	4	3	1789	1806	43
2	4	3	1475	1563	44
4	4	3	1135	1156	31
1	5	3	2492	2532	31
3	5	3	1923	1967	35
5	5	3	1328	1350	30
0	6	3	2278	2212	44
2	6	3	1933	1927	45
4	6	3	1381	1401	30
1	7	3	201	217	116
3	7	3	0	183	1
0	8	3	953	956	32
2	8	3	873	846	39
4	8	3	683	638	47
1	9	3	1738	1714	26
3	9	3	1389	1411	33
0	10	3	503	469	55
2	10	3	345	438	107
1	11	3	1182	1211	57
3	11	3	1100	1039	38
0	12	3	1430	1386	29
2	12	3	1257	1278	36
1	13	3	1280	1250	84
0	0	4	3625	3578	36
2	0	4	3131	3068	36
4	0	4	2241	2202	26
1	1	4	1210	1166	25
3	1	4	952	921	17
5	1	4	653	656	33
0	2	4	191	262	96
2	2	4	240	209	109
4	2	4	94	136	94
1	3	4	0	38	1
3	3	4	0	28	1
5	3	4	191	9	190
0	4	4	590	602	36
2	4	4	572	528	49
4	4	4	404	381	60
1	5	4	301	214	56
3	5	4	436	155	74
5	5	4	334	116	97
0	6	4	762	829	37
2	6	4	781	752	41
4	6	4	610	583	50
1	7	4	2405	2443	26
3	7	4	1974	2011	32
0	8	4	911	924	35
2	8	4	885	846	39
4	8	4	617	669	60
1	9	4	286	65	74
3	9	4	248	58	248
0	10	4	354	296	82
2	10	4	427	277	81
1	11	4	676	679	34
0	12	4	270	62	142
1	1	5	1377	1361	17
3	1	5	1049	1062	20
5	1	5	756	717	27
0	2	5	1668	1677	40
2	2	5	1498	1446	39
4	2	5	1104	1025	27
1	3	5	2994	2981	38
3	3	5	2332	2390	33
0	4	5	2692	2741	38
2	4	5	2419	2443	42
4	4	5	1809	1847	26
1	5	5	1232	1182	60
3	5	5	921	929	38
0	6	5	1086	1104	30
2	6	5	936	982	42
4	6	5	740	726	48
1	7	5	742	726	26
3	7	5	611	604	56
0	8	5	1059	1036	32
2	8	5	955	937	42
1	9	5	1103	1105	23
3	9	5	890	929	49
0	10	5	2071	1982	27
2	10	5	1729	1825	35
1	11	5	1448	1428	24
0	0	6	2852	2806	33
2	0	6	2493	2513	41
4	0	6	1910	1915	24
1	1	6	889	858	12
3	1	6	712	718	24
0	2	6	337	175	65
2	2	6	268	151	151
4	2	6	139	117	139
1	3	6	319	90	45
3	3	6	153	65	153
0	4	6	606	561	37
2	4	6	479	503	72
4	4	6	402	377	82
1	5	6	195	213	123
3	5	6	256	176	192
0	6	6	666	687	41
2	6	6	662	631	53
1	7	6	2079	2072	45
3	7	6	1695	1753	36
0	8	6	705	698	44
2	8	6	685	646	60
1	9	6	0	17	1
0	10	6	300	249	122
1	1	7	1353	1320	15
3	1	7	1111	1090	22
0	2	7	1750	1824	31
2	2	7	1682	1649	38
4	2	7	1262	1268	33
1	3	7	876	845	24
3	3	7	680	725	56
0	4	7	1116	1127	26
2	4	7	1059	1038	40
1	5	7	1668	1651	25
3	5	7	1426	1385	38
0	6	7	1417	1421	30
2	6	7	1314	1303	39
1	7	7	194	177	193
0	8	7	663	677	50
2	8	7	675	627	64
1	9	7	1251	1219	36
0	0	8	248	322	105
2	0	8	229	308	200
1	1	8	1811	1802	12
3	1	8	1513	1524	22
0	2	8	289	171	81
2	2	8	0	153	1
1	3	8	1374	1391	20
3	3	8	1152	1181	47
0	4	8	1099	1156	30
2	4	8	1064	1061	45
1	5	8	417	405	48
0	6	8	1291	1278	31
2	6	8	1156	1180	48
1	7	8	395	257	56
1	1	9	64	85	64
0	2	9	0	35	1
2	2	9	355	34	124
1	3	9	1290	1318	21
0	4	9	1342	1359	30

Supplementary information: additional bond lengths (Å) and angles (°)

In-Pd#1	2.783(2)	In-Pd#2	2.8421(9)
In-Pd#3	2.8421(9)	In-In#4	2.973(2)
In-In#5	3.064(2)	In-Ce#6	3.2891(9)
In-Ce#7	3.2891(9)	In-Ce#8	3.396(2)
In-Ce#2	3.5786(13)	In-Ce#3	3.5786(13)
Ce-Pd	3.021(3)	Ce-Pd#9	3.278(2)
Ce-Pd#10	3.278(2)	Ce-In#11	3.2891(9)
Ce-In#12	3.2891(9)	Ce-In#13	3.2891(9)
Ce-In#14	3.2891(9)	Ce-In#15	3.396(2)
Ce-In#8	3.396(2)	Ce-In#2	3.5786(13)
Ce-In#16	3.5786(13)	Ce-In#17	3.5786(13)
Pd-In#18	2.783(2)	Pd-In#4	2.783(2)
Pd-In#17	2.8421(9)	Pd-In#2	2.8421(9)
Pd-In#3	2.8421(9)	Pd-In#16	2.8421(9)
Pd-Ce#19	3.278(2)	Pd-Ce#20	3.278(2)

Pd#1-In-Pd#2	105.63(3)	Pd#1-In-Pd#3	105.63(3)
Pd#2-In-Pd#3	108.77(5)	Pd#1-In-In#4	143.65(4)
Pd#2-In-In#4	58.47(2)	Pd#3-In-In#4	58.47(2)
Pd#1-In-In#5	112.10(6)	Pd#2-In-In#5	112.15(5)
Pd#3-In-In#5	112.15(5)	In#4-In-In#5	104.26(4)
Pd#1-In-Ce#6	64.73(4)	Pd#2-In-Ce#6	168.55(4)
Pd#3-In-Ce#6	80.67(2)	In#4-In-Ce#6	132.95(2)
In#5-In-Ce#6	68.46(3)	Pd#1-In-Ce#7	64.73(4)
Pd#2-In-Ce#7	80.67(2)	Pd#3-In-Ce#7	168.55(4)
In#4-In-Ce#7	132.95(2)	In#5-In-Ce#7	68.46(3)
Ce#6-In-Ce#7	89.25(3)	Pd#1-In-Ce#8	79.60(4)
Pd#2-In-Ce#8	62.67(4)	Pd#3-In-Ce#8	62.67(4)
In#4-In-Ce#8	64.05(2)	In#5-In-Ce#8	168.30(6)
Ce#6-In-Ce#8	118.89(3)	Ce#7-In-Ce#8	118.89(3)
Pd#1-In-Ce#2	135.59(2)	Pd#2-In-Ce#2	54.69(5)
Pd#3-In-Ce#2	118.15(4)	In#4-In-Ce#2	65.46(2)
In#5-In-Ce#2	58.75(3)	Ce#6-In-Ce#2	127.21(3)
Ce#7-In-Ce#2	72.40(2)	Ce#8-In-Ce#2	113.23(3)
Pd#1-In-Ce#3	135.59(2)	Pd#2-In-Ce#3	118.15(4)
Pd#3-In-Ce#3	54.69(5)	In#4-In-Ce#3	65.46(2)
In#5-In-Ce#3	58.75(3)	Ce#6-In-Ce#3	72.40(2)
Ce#7-In-Ce#3	127.21(3)	Ce#8-In-Ce#3	113.23(3)
Ce#2-In-Ce#3	80.43(4)	Pd-Ce-Pd#9	135.19(3)
Pd-Ce-Pd#10	135.19(3)	Pd#9-Ce-Pd#10	89.62(6)
Pd-Ce-In#11	101.87(3)	Pd#9-Ce-In#11	50.14(2)
Pd#10-Ce-In#11	110.44(4)	Pd-Ce-In#12	101.87(3)
Pd#9-Ce-In#12	110.44(4)	Pd#10-Ce-In#12	50.14(2)
In#11-Ce-In#12	156.27(6)	Pd-Ce-In#13	101.87(3)
Pd#9-Ce-In#13	50.14(2)	Pd#10-Ce-In#13	110.44(4)
In#11-Ce-In#13	85.90(3)	In#12-Ce-In#13	89.25(3)
Pd-Ce-In#14	101.87(3)	Pd#9-Ce-In#14	110.44(4)
Pd#10-Ce-In#14	50.14(2)	In#11-Ce-In#14	89.25(3)
In#12-Ce-In#14	85.90(3)	In#13-Ce-In#14	156.27(6)
Pd-Ce-In#15	154.05(2)	Pd#9-Ce-In#15	50.36(3)
Pd#10-Ce-In#15	50.36(3)	In#11-Ce-In#15	61.11(3)
In#12-Ce-In#15	96.51(3)	In#13-Ce-In#15	96.51(3)
In#14-Ce-In#15	61.11(3)	Pd-Ce-In#8	154.05(2)
Pd#9-Ce-In#8	50.36(3)	Pd#10-Ce-In#8	50.36(3)
In#11-Ce-In#8	96.51(3)	In#12-Ce-In#8	61.11(3)

In#13-Ce-In#8	61.11(3)	In#14-Ce-In#8	96.51(3)
In#15-Ce-In#8	51.91(4)	Pd-Ce-In#2	50.15(2)
Pd#9-Ce-In#2	155.46(2)	Pd#10-Ce-In#2	89.98(3)
In#11-Ce-In#2	150.26(4)	In#12-Ce-In#2	52.79(3)
In#13-Ce-In#2	107.60(2)	In#14-Ce-In#2	87.78(2)
In#15-Ce-In#2	139.28(2)	In#8-Ce-In#2	113.23(3)
Pd-Ce-In#16	50.15(2)	Pd#9-Ce-In#16	155.46(2)
Pd#10-Ce-In#16	89.98(3)	In#11-Ce-In#16	107.60(2)
In#12-Ce-In#16	87.78(2)	In#13-Ce-In#16	150.26(4)
In#14-Ce-In#16	52.79(3)	In#15-Ce-In#16	113.23(3)
In#8-Ce-In#16	139.28(2)	In#2-Ce-In#16	49.08(4)
Pd-Ce-In#17	50.15(2)	Pd#9-Ce-In#17	89.98(3)
Pd#10-Ce-In#17	155.46(2)	In#11-Ce-In#17	52.79(3)
In#12-Ce-In#17	150.26(4)	In#13-Ce-In#17	87.78(2)
In#14-Ce-In#17	107.60(2)	In#15-Ce-In#17	113.23(3)
In#8-Ce-In#17	139.28(2)	In#2-Ce-In#17	100.30(5)
In#16-Ce-In#17	80.43(4)	In#18-Pd-In#4	107.29(7)
In#18-Pd-In#17	124.96(3)	In#4-Pd-In#17	74.37(3)
In#18-Pd-In#2	74.37(3)	In#4-Pd-In#2	124.96(3)
In#17-Pd-In#2	150.32(9)	In#18-Pd-In#3	74.37(3)
In#4-Pd-In#3	124.96(3)	In#17-Pd-In#3	63.07(4)
In#2-Pd-In#3	108.77(5)	In#18-Pd-In#16	124.96(3)
In#4-Pd-In#16	74.37(3)	In#17-Pd-In#16	108.77(5)
In#2-Pd-In#16	63.07(4)	In#3-Pd-In#16	150.32(9)
In#18-Pd-Ce	126.35(4)	In#4-Pd-Ce	126.35(4)
In#17-Pd-Ce	75.16(4)	In#2-Pd-Ce	75.16(4)
In#3-Pd-Ce	75.16(4)	In#16-Pd-Ce	75.16(4)
In#18-Pd-Ce#19	65.13(3)	In#4-Pd-Ce#19	65.13(3)
In#17-Pd-Ce#19	138.99(5)	In#2-Pd-Ce#19	66.97(3)
In#3-Pd-Ce#19	138.99(5)	In#16-Pd-Ce#19	66.97(3)
Ce-Pd-Ce#19	135.19(3)	In#18-Pd-Ce#20	65.13(3)
In#4-Pd-Ce#20	65.13(3)	In#17-Pd-Ce#20	66.97(3)
In#2-Pd-Ce#20	138.99(5)	In#3-Pd-Ce#20	66.97(3)
In#16-Pd-Ce#20	138.99(5)	Ce-Pd-Ce#20	135.19(3)
Ce#19-Pd-Ce#20	89.62(6)		

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 -x-1/2,-y+1/2,-z+1 #3 -x+1/2,-y+1/2,-z+1

#4 x,y,-z+3/2 #5 -x,-y,-z+2 #6 x+1/2,y-1/2,z+1

#7 x-1/2,y-1/2,z+1 #8 -x,-y+1,-z+1 #9 x+1/2,y+1/2,z

#10 x-1/2,y+1/2,z #11 x+1/2,y+1/2,-z+3/2 #12 x-1/2,y+1/2,z-1

#13 x+1/2,y+1/2,z-1 #14 x-1/2,y+1/2,-z+3/2 #15 -x,-y+1,z-1/2

#16 -x-1/2,-y+1/2,z-1/2 #17 -x+1/2,-y+1/2,z-1/2 #18 x,y,z-1

#19 x-1/2,y-1/2,z #20 x+1/2,y-1/2,z

**************************end page 6*********************************

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